the free energies of solvation of model compounds closer to experimental values. Further research will involve evaluating the radius of gyration of PEG in salt solutions to improve the interaction of ether oxygens with ions in simulation (*Colloid Jour.*, ***72(2):*** 279 - 281).

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Simulation of Linoleoyl-Containing Pure Lipid Bilayer and Soybean Plasma Membranes

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Molecular dynamics (MD) simulations have been extensively used to study lipid membranes in addition to experimental studies as they help better understand membranes in the atomic level. Computational models of bacterial (*E. coli*) membranes have been developed and applied to study the antimicrobial peptide proteins. Plant membranes are less frequently studied compared to the bacterial membrane. In this work, we will present the soybean plasma membranes models. The compositions of cell plasma membranes of soybean vary depending on the species, stage of development, and the part of the plant. The two parts of the plant that we study are the hypocotyl and the root. Each model consists of 100 lipids per leaflet, with the composition based on the weighted and averaged values from past experimental studies. Specifically, the hypocotyl membrane contains 7 types of unsaturated phospholipids and two types of sterols, while the root membrane contains 8 types of phospholipids and two types of sterols. All types of phospholipids in soybean contains the 18:2 (cis Δ9, 12) linoleoyl tail which was not well studied before, therefore, the simulations on the pure 18:0/18:2 and 18:2/18:2 phosphocholine (PC) lipid bilayers are also performed. The structural properties such as surface area per lipid, bilayer thicknesses, order parameters, and spin-lattice relaxation time are analyzed for all membranes. Moreover, the analyses of the sterols tilt angle distributions, hydrogen bonding, and clustering are also conducted for the soybean membranes. The structural properties of pure bilayers agree well with NMR experimental data validate the accuracy of 18:2 linoleoyl-containing lipids, based on which the soybean membrane models also result in reasonable structural properties. These results imply that the two soybean membrane models are realistic, and can facilitate the further study of soybean and other plant membranes.

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Lateral Heterogeneity of Cholesterol on Binary Lipid Mixtures of POPC/Chol Imaged with AFM

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Phase diagrams on ternary and quaternary lipid mixtures showing the existence of liquid-ordered (lo), liquid-disordered (ld) and a mixed phase (lo+ld) are now well established. However the existence of such a phase diagram on binary mixtures is still in debate despite reports of a phase diagram on the mixtures POPC/Chol and POPC/Erg and nystatin activity co-related to this purported phase diagram; with a maximal activity appearing in the mixed phase. Recent Molecular Dynamics simulations of POPC/Chol at different temperatures and cholesterol concentrations along this phase diagram, suggest the existence of cholesterol enriched nanosites in this mixed phase, indicating the presence of cholesterol lateral heterogeneity. Here we present atomic force microscopy images of supported lipid bilayers made up of POPC and different cholesterol concentrations along the phase diagram. We observe structures that are consistent with the Molecular Dynamics predictions of order parameters and membrane thickness, supporting the idea of cholesterol lateral heterogeneity in binary mixtures, which can enrich the discussion on the existence of lipid rafts and domains in biological membranes. *Funding: DGAPA-PAPIIT-RG100416.*

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Orientational Properties of DOPC/SM/Cholesterol Mixtures: A PM-IRRAS Study

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Sphingomyelins (SM) and phosphatidylcholines (PC) are major lipid classes in the external plasma membrane leaflet of mammalian cells. A preferential interaction between SM and cholesterol (Cho) in both cell and model membranes has been proposed as central for the formation of Cho- and SM-rich domains in membranes. In this context, the relevance of the SM hydrophobic moiety on its interaction with Cho for domain stabilization has been investigated by our group (1-2). We report here on the effects of sphingomyelin structure on the orientational and conformational properties of monolayers of pure lipids and of two ternary lipid mixtures (DOPC/16:0SM/Cho and DOPC/24:1SM/Cho), which are relevant as mammalian cell membrane models. We investigated interchain interactions, hydrogen bonding, conformational and structural properties using *in situ* polarization-modulated infrared reflection absorption spectroscopy (PM-IRRAS). Our results indicate that the particular properties conferred on sphingolipids by unsaturation have profound implications on membrane organization. Finally, we also explored the orientational and conformational changes in lipid monolayers of DOPC/16:0SM/Cho 2:1:1 after the adsorption/insertion of the active toxin HlyA and its unacylated nonhemolytic precursor ProHlyA, so as to complement our knowledge on the action mechanism of both proteins.

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Investigating Lipid Domain Formation in Asymmetric Large Unilamellar Vesicles using Förster Resonance Energy Transfer (FRET)

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Many living cell membranes display lipid asymmetry, with a distinct difference between the phospholipid and sphingolipid compositions of the inner and outer leaflets of the lipid bilayer. We recently developed improved methods to prepare asymmetric lipid vesicles using using alpha-cyclodextrins. These hexasaccharide rings can promote the exchange of lipids between vesicles, but do not transport sterols. This allows the efficient and selective replacement of the outer leaflet lipids of lipid vesicles without perturbing sterol content. Here we show, using several types of asymmetric vesicles, it is possible to investigate ordered domain formation in both the inner and outer leaflets of large unilamellar vesicles using FRET. To do this, large unilamellar vesicles are prepared with FRET acceptor probes in either only the inner or only the outer leaflet. FRET was used to study cholesterol-containing vesicles in which sphingomyelin was the predominant lipid in either the inner leaflet or the outer leaflet, and the opposite leaflet was composed of unsaturated phosphatidylethanolamine and phosphatidylserine, or of unsaturated phosphatidylcholine. Preliminary results show that in at least some of the lipid compositions studied ordered lipid domains in one leaflet can induce ordered lipid domains in leaflets composed of lipids which do not normally form ordered domains by themselves. These results support the findings of our previous studies of domain formation and interleaflet coupling using microscopy, and show that the FRET approach can be extended to study interleaflet coupling in membranes containing submicroscopic domains.

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Lipid Mixing in Model Membranes

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The plasma membrane constitutes the boundary between the cell and its environment. It is believed to have a highly organized lateral structure (the raft hypothesis). Due to the complex composition of plasma membranes, model lipid bilayers of simple composition are often used in experiments and simulations to study the lateral organization. Here we conducted all-atom (AA) and coarse-grained (CG) simulations of bilayers containing POPC, POPC:cholesterol, DPPC:DOPC, DPPC:DOPC:cholesterol and